

# Mott transition at large orbital degeneracy: dynamical mean-field theory

S. Florens,<sup>1</sup> A. Georges,<sup>1</sup> G. Kotliar,<sup>2</sup> and O. Parcollet<sup>3</sup>

<sup>1</sup>*Laboratoire de Physique Théorique, Ecole Normale Supérieure,  
24 rue Lhomond, 75231 Paris Cedex 05, France*

*and Laboratoire de Physique des Solides, Université Paris-Sud, Bât. 510, 91405 Orsay, France*

<sup>2</sup>*Center for Materials Theory, Department of Physics and Astronomy,  
Rutgers University, Piscataway, NJ 08854, USA*

<sup>3</sup>*Service de Physique Théorique, CEA Saclay, 91191 Gif-Sur-Yvette, France*  
(Dated: May 13th, 2002)

We study analytically the Mott transition of the  $N$ -orbital Hubbard model using dynamical mean-field theory and a low-energy projection onto an effective Kondo model. It is demonstrated that the critical interaction at which the insulator appears ( $U_{c1}$ ) and the one at which the metal becomes unstable ( $U_{c2}$ ) have different dependence on the number of orbitals as the latter becomes large:  $U_{c1} \propto \sqrt{N}$  while  $U_{c2} \propto N$ . An exact analytical determination of the critical coupling  $U_{c2}/N$  is obtained in the large- $N$  limit. The metallic solution close to this critical coupling has many similarities at low-energy with the results of slave boson approximations, to which a comparison is made. We also discuss how the critical temperature associated with the Mott critical endpoint depends on the number of orbitals.

## I. INTRODUCTION

The Mott transition is one of the central problems in the field of strongly correlated electronic systems. It is directly relevant to many compounds, such as  $V_2O_3$ ,  $NiS_{2-x}Se_x$  [1], fullerenes [2], and two-dimensional organics of the  $\kappa$ -BEDT family [3]. Viewed from a more general perspective, the Mott transition confronts us with the need to describe electrons in a solid in an intermediate coupling regime, where perturbative methods around either the localised or the itinerant limit are of very limited use. The Mott phenomenon is also a key issue for the development of electronic structure calculations of strongly correlated materials, a subject of current intense investigation [4].

A breakthrough in the understanding of this problem resulted from the development of dynamical mean-field theory (DMFT) [5, 6, 7, 8]. Following the observation that a Mott transition as a function of the interaction strength  $U$  takes place in a (fully frustrated) one-band Hubbard model at half-filling [9] within DMFT, a rather surprising scenario was unravelled [10]. In the parameter space defined by temperature and interaction strength, two kinds of solutions of the DMFT equations were found, corresponding to an insulator and a metal, with a region  $U_{c1}(T) < U < U_{c2}(T)$  in which both types of solution coexist. The spectral function of the insulating solution has only high-energy features corresponding to Hubbard bands, while the metallic solution also has a low-energy quasiparticle resonance. Coexistence results in a *first-order* phase transition at finite temperature. The first order line ends into a second-order critical endpoint at  $T = T_{MIT}$ ,  $U = U_{MIT}$  at which the coexistence domain closes ( $U_{c1}(T_{MIT}) = U_{c2}(T_{MIT}) = U_{MIT}$ ). At  $T = 0$ , the transition is also second-order, because the metallic solution always has lower energy than the in-

ulating one. A qualitative picture of the evolution of the spectral function as a function of control parameters was obtained, and this resulted in successful experimental predictions [11].

Early work on these issues relied heavily on an accurate but approximate technique, the iterative perturbation theory [6, 10]. Later on, exact results near  $U_{c2}(T = 0)$  were obtained [12, 13], thanks to the development of a renormalization method exploiting the separation of energy scales that holds true close to this critical coupling. This method performs a projection onto a low-energy effective theory after elimination of the degrees of freedom corresponding to Hubbard bands. A clear picture of the structure of the DMFT equations near the Mott transition and of the different critical points was finally obtained through the introduction of a Landau functional approach [14]. These established results for the one-band Hubbard model together with numerical methods for solving DMFT equations, such as Quantum Monte Carlo [9, 15] and Numerical Renormalization Group [16], provide now a consistent picture of the Mott transition within DMFT.

In this paper, we investigate the Mott transition in the limit of large orbital degeneracy, within DMFT. We establish analytically that the critical couplings  $U_{c1}(T = 0)$  and  $U_{c2}(T = 0)$  are not only different, but that they have very different scalings as a function of the number  $N$  of orbitals. Indeed,  $U_{c1}$  increases as  $\sqrt{N}$ , while  $U_{c2}$  increases as  $N$ , so that the coexistence region widens. Close to  $U_{c2}$ , the separation of scales which is at the heart of the projective method becomes asymptotically exact for large  $N$ . This allows us to determine exactly the value of the critical coupling  $U_{c2}/N$  at large  $N$ , and also to demonstrate that slave-boson like approximations become asymptotically valid at low energy in this limit. Finally, we discuss how the finite temperature metal-

insulator transition depends on the number of orbitals.

Our findings on the critical couplings are in agreement with early QMC results for the two-orbital model ( $N = 4$ ) [21], and with recent results for higher values of  $N$  [22]. A widening of the coexistence window  $[U_{c1}, U_{c2}]$  as  $N$  increases is clearly seen in these simulations. Also, for fixed  $N$ , the critical coupling required to enter the Mott state is largest [18] at the particle-hole symmetric filling  $n = 1/2$ . The present work also puts the results of Refs.[19, 20] in a new perspective: there, a  $\sqrt{N}$  scaling of the critical coupling was proposed. We find that this indeed applies to the coupling where the insulator becomes unstable ( $U_{c1}$ ), while the true  $T = 0$  Mott transition (at which the quasiparticle residue vanishes) takes place at  $U_{c2} \propto N$ . Indeed, in Ref.[19], the  $\sqrt{N}$  scaling was rationalized on the basis of a stability argument for the insulator. Finally, the rather high temperatures considered in [20] explain why only the  $\sqrt{N}$  dependence was reported there: distinguishing  $U_{c2}$  from  $U_{c1}$  requires significantly lower temperatures [22].

The limit of large orbital degeneracy is relevant to the physics of systems with partially filled d- or f- shells, as well as to fullerenes. Direct numerical approaches become prohibitively difficult as the number of orbital increases (QMC methods scale as a power law of  $N$ , while exact diagonalizations [17] scale exponentially). It is therefore important for future research to develop approximate but accurate impurity solvers which can handle many orbitals. The controlled results that we establish in this paper can be used as tests of these approximation methods.

## II. MULTI-ORBITAL HUBBARD MODEL

We consider a generalized Hubbard model involving  $N$  species of electrons, with Hamiltonian:

$$H = - \sum_{i,j} \sum_{\sigma=1}^N t_{ij} d_{i\sigma}^\dagger d_{j\sigma} + \frac{U}{2} \sum_i \left[ \sum_{\sigma=1}^N \left( d_{i\sigma}^\dagger d_{i\sigma} - n \right) \right]^2 - \tilde{\mu} \sum_i \sum_{\sigma=1}^N d_{i\sigma}^\dagger d_{i\sigma} \quad (1)$$

where  $i, j$  are sites indices,  $\sigma$  the orbital index,  $\tilde{\mu}$  is the chemical potential and  $n$  the average density of particles per species :

$$n = \frac{1}{N} \sum_{\sigma} \langle d_{i\sigma}^\dagger d_{i\sigma} \rangle \quad (2)$$

Introducing  $n$  in the Hamiltonian is just a convention for the chemical potential  $\tilde{\mu}$ . In particular, it is convenient at half-filling where the particle-hole symmetry implies  $n = \frac{1}{2}$  and  $\tilde{\mu} = 0$ . For a single site (atom), the spectrum consists of  $N+1$  levels, with energies  $\frac{U}{2}(Q-nN)^2$  depending only on the total charge on the orbital:  $Q = 0, \dots, N$  and with degeneracies  $\binom{N}{Q}$ .

The usual single-orbital Hubbard model corresponds to  $N = 2$  ( $\sigma = \uparrow, \downarrow$ ). The Hamiltonian considered here has a full  $SU(N)$  symmetry which includes both spin and orbital degrees of freedom. Starting from a more realistic model which assumes an interaction matrix  $U_{mm'}$  between opposite spins and  $U_{mm'} - J_{mm'}$  between parallel spins, it corresponds to the limit of isotropic  $U_{mm'} = U$  and vanishing Hund's coupling  $J_{mm'} = 0$ .

When  $U$  is large enough, we expect a Mott insulating state to exist at fillings  $n = Q/N$ , corresponding to an integer occupancy of each site on average  $Q = 1, \dots, N-1$ . In this paper, we investigate analytically the nature of these Mott transitions within DMFT. We consider only phases with no magnetic ordering and study the transition between a paramagnetic metal and a paramagnetic Mott insulator. In Section III, we extract the large- $N$  behaviour of  $U_{c1}$  and  $U_{c2}$  using the low-energy projective technique analysis of the DMFT equations introduced in [12] for  $N = 2$  and extended in [23] : we show that the equations for the  $U_c$ 's derived by this method are greatly simplified for  $N \rightarrow \infty$  in the sense that an atomic limit becomes exact. In section IV, we find quantitative agreement between these results and a multiorbital slave boson method. Finally, in Sec.V, we consider the Mott transition at finite temperature.

## III. LARGE- $N$ BEHAVIOUR OF $U_{c1}$ AND $U_{c2}$

### A. DMFT and the low-energy projective method

Let us recall briefly the DMFT equations and their low-energy projective analysis [12, 13]. DMFT maps the lattice Hamiltonian above onto a multi-orbital Anderson impurity model with the same local interaction term than in (1) and a hybridization function  $\Delta(i\omega_n)$ . The local Green's function reads:  $G_d(i\omega_n)^{-1} = i\omega_n + \tilde{\mu} - \Delta(i\omega_n) - \Sigma_d(i\omega_n)$ . In this expression,  $\tilde{\mu}$  is the chemical potential (shifted by the Hartree contribution) and  $\Sigma_d(i\omega_n)$  is a local self-energy. A self-consistency requirement is imposed, which identifies  $G_d(i\omega_n)$  with the on-site Green's function of the lattice model with the same self-energy  $\Sigma_d(i\omega_n)$ . This reads:

$$G_d(i\omega_n) = \int d\varepsilon \frac{D(\varepsilon)}{i\omega_n + \tilde{\mu} - \varepsilon - \Sigma_d(i\omega_n)} \quad (3)$$

In this expression,  $D(\varepsilon)$  is the free electron density of state (d.o.s.) corresponding to the Fourier transform of the hopping matrix elements  $t_{ij}$ . In the particular case of a semi-circular d.o.s. with half-width  $D = 2t$ , equation (3) simplifies to:

$$\Delta(i\omega_n) = t^2 G_d(i\omega_n) \quad (4)$$

Solving the impurity model subject to (3) determines both the hybridization function and the local Green's function in a self-consistent manner. In order to give an explicit Hamiltonian form to the Anderson impurity

model, the function  $\Delta$  can be represented with an auxiliary bath of conduction electrons  $c_{k\sigma}$ , with effective single-particle energies  $\epsilon_k$  and effective hybridizations  $V_k$  to the local orbital such that :

$$\Delta(i\omega) \equiv \sum_k \frac{|V_k|^2}{i\omega - \epsilon_k} \quad (5)$$

$$H = \sum_{k\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{k,\sigma} V_k (c_{k,\sigma}^\dagger d_\sigma + d_\sigma^\dagger c_{k,\sigma}) - \tilde{\mu} \sum_\sigma d_\sigma^\dagger d_\sigma + \frac{U}{2} \left[ \sum_\sigma (d_\sigma^\dagger d_\sigma - n) \right]^2 \quad (6)$$

Within DMFT, the Mott transition at  $U_{c2}$  and  $T = 0$  is associated with a separation of energy scales. For  $U$  slightly smaller than  $U_{c2}$ , the d-electron spectral function has a sharp quasiparticle peak, well separated from the high-energy Hubbard bands. Naturally, a small amount of spectral weight does connect these two features in the metal. Slightly above  $U_{c2}$ , the Mott gap  $\Delta_g$  separating the Hubbard bands of the insulating solution is finite. While the weight  $Z$  of the quasiparticle peak vanishes at  $U_{c2}$ , the Mott gap  $\Delta_g$  disappears only at the smaller critical coupling  $U_{c1}$ . Because of the self-consistency condition (3), the hybridization function of the effective conduction bath (and hence the  $\epsilon_k$ 's) also displays this separation of scales.

This remark led the authors of Ref. [12] to use a *projective method* in order to study the critical behaviour at  $U_{c2}$ . Within this approach, the effective conduction electron bath is separated into a high energy sector ( $k \in H^\pm$ ) associated with the upper ( $H^+$ ) and lower ( $H^-$ ) Hubbard bands, and a low-energy sector ( $k \in L$ ) associated with the quasiparticle resonance. The impurity model Hamiltonian is thus written as (for simplicity we take  $V_L$  and  $V_H$  independent of  $k$ ):

$$H = H_L + H_H + H_{HL} \quad (7a)$$

$$H_L = \sum_{k \in L, \sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} \quad (7b)$$

$$H_H = \sum_{k \in H^\pm, \sigma} \left[ \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + V_H c_{k,\sigma}^\dagger d_\sigma + h.c. \right] + \frac{U}{2} \left[ \sum_\sigma d_\sigma^\dagger d_\sigma - n \right]^2 - \tilde{\mu} \sum_\sigma d_\sigma^\dagger d_\sigma \quad (7c)$$

$$H_{HL} = \sum_{k \in L, \sigma} \left[ V_L c_{k,\sigma}^\dagger d_\sigma + h.c. \right] \quad (7d)$$

We note that the self-consistency condition (3) implies that  $\sum_{k \in L} V_L^2/t^2$  is proportional to the quasi-particle residue  $Z$ , so that it is clear that the low-energy hybridization vanishes at  $U_{c2}$ .

In order to obtain an effective theory close to  $U_{c2}$ , one first diagonalizes the high-energy part  $H_H$  of the Hamiltonian, and obtains an effective low-energy hamiltonian by expanding in  $V_L$ . From the presence of a finite gap in

the high-energy bath  $\epsilon_k$  (for  $k \in H^\pm$ ),  $H_H$  describes an impurity in a semiconducting bath. The position of the d-level (*i.e.* the chemical potential) fixes the number of electrons in the ground-state. For a charge  $Q = nN$ , this high-energy problem has a  $\binom{N}{Q}$  degenerate ground-state, spanned by eigenvectors  $|\mu\rangle$  (with eigen-energy  $E_{gs}$ ). The detailed form of these states is complicated (they mix with higher impurity charge states through  $V_H$ ), but *they form a representation of the  $SU(N)$  "spin" group, of dimension  $\binom{N}{Q}$ .*

Using a generalized Schrieffer-Wolff (SW) transformation to order  $V_L^2$  in order to project onto the low-energy Hilbert space (defined by the selected charge sector of the impurity  $d$ , and the low-energy sector for the conduction bath  $k \in L$ ), one obtains an effective Kondo Hamiltonian [12, 13, 23] :

$$H_{\text{eff}} = \sum_{k \in L, \sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \frac{V_L^2}{U} \sum_{kk', \mu\nu, \sigma\sigma'} J_{\mu\nu}^{\sigma\sigma'} X^{\mu\nu} c_{k,\sigma}^\dagger c_{k',\sigma'} \quad (8)$$

where  $X^{\mu\nu} \equiv |\mu\rangle\langle\nu|$  is a Hubbard operator connecting two states in the ground state manifold. The Hamiltonian contains potential scattering terms for  $\sigma = \sigma'$  and spin-flip (Kondo) terms for  $\sigma \neq \sigma'$ , with the spin operator  $S_{\mu\nu} = X^{\mu\nu} - \delta_{\mu\nu} X^{\rho\rho}$ . The matrix of (dimensionless) coupling constants reads [13, 23]:

$$J_{\mu\nu}^{\sigma\sigma'} \equiv \left\langle \mu \left| d_{\sigma'}^\dagger \frac{U}{H_H - E_{gs}} d_\sigma \right| \nu \right\rangle - \left\langle \mu \left| d_\sigma \frac{U}{H_H - E_{gs}} d_{\sigma'}^\dagger \right| \nu \right\rangle \quad (9)$$

We emphasize that the low-energy Hamiltonian has been derived to first order in  $V_L^2$ : this is asymptotically justified exactly at the critical point (and hence sufficient to determine the critical coupling), but deviations away from the critical point require to consider higher order terms in  $V_L$ . Finally, we note that the bandwidth of this Kondo problem is of order  $Zt$ , while the coupling is of order  $V_L^2/U \sim Zt^2/U$ . Hence, the dimensionless coupling constant of the effective low-energy Kondo problem is of order one: we have an *intermediate coupling* Kondo problem [14].

The conditions that determine  $U_{c1}$  and  $U_{c2}$  have been derived within the projective method [12, 23] and within the more general Landau functional approach [14] (in which the stability of the insulating solution to different kinds of low-energy perturbations is studied using a Landau functional of the hybridization function  $\Delta(i\omega_n)$ ). The condition for  $U_{c2}$  reads:

$$\frac{U_{c2}^2}{t^2} = \sum_{\alpha\beta\mu\nu} \binom{N}{nN}^{-1} |J_{\mu\nu}^{\alpha\beta}|^2 + \langle X_{\mu\nu} c_\alpha^\dagger c_\beta \rangle \left( J_{\rho\nu}^{\gamma\beta} J_{\rho\mu}^{\alpha*} - J_{\mu\rho}^{\gamma\beta} J_{\nu\rho}^{\alpha*} \right) \quad (10)$$

As explained in [14, 23], an analogous equation is found for  $U_{c1}$ , where off-diagonal terms in the average are taken

to zero. For finite  $N$ , this equation is complicated to solve, since the average on the right-hand side is a function of  $J$  which we can only obtain by solving the low energy Kondo problem explicitly. However, we will show in the following that :

1. Using the  $SU(N)$  symmetry, the tensor structure of  $J$  can be parametrized with only two numbers  $A$  and  $B$ , which are dimensionless functions of  $N$ ,  $n$ , and  $V_H/U$ . This greatly simplifies (10) (Section IIIB).
2. An explicit calculation of  $A$  and  $B$  can be performed in the atomic limit  $V_H = 0$ . This allows us to show that the two critical couplings have the following  $N$ -dependence at large  $N$ :

$$U_{c1} = \sqrt{N} \tilde{U}_{c1} + \dots \quad (11a)$$

$$U_{c2} = N \tilde{U}_{c2} + \dots \quad (11b)$$

In fact, the atomic limit evaluation of  $A$  and  $B$  becomes asymptotically exact when  $U$  is taken to be proportional to  $N$ . This is not the case when  $U \propto \sqrt{N}$ , but we show that corrections to the atomic limit do not modify the scaling (11a).

3. For  $U \propto N$ , the effective Kondo problem can actually be solved explicitly at large  $N$ , using standard techniques. This allows for an explicit computation of the matrix element  $\langle X_{\mu\sigma} c_{\alpha}^{\dagger} c_{\beta} \rangle$  involved in (10). Since, from the above remark, the effective couplings entering the Kondo problem can be evaluated in the atomic limit in that case, this allows us to determine the prefactor  $\tilde{U}_{c2}$  exactly (Sec. IIID). Because the atomic limit is not asymptotically exact for  $U \propto \sqrt{N}$ , we are not able to obtain an exact determination of  $\tilde{U}_{c1}$ .

### B. Simplification due to the $SU(N)$ symmetry

Computing the couplings (9) is a complicated task in general, since it requires a knowledge of the states  $|\mu\rangle, |\nu\rangle$ , and thus a diagonalization of  $H_H$ . However, general considerations based on the  $SU(N)$  symmetry of the model allow one to reduce the unknown Kondo couplings  $J_{\mu\sigma}^{\sigma\sigma'}$  to two dimensionless numbers only. Let us consider the operator:

$$O_1^{\sigma\sigma'} \equiv d_{\sigma} \frac{1}{H_H - E_{gs}} d_{\sigma'}^{\dagger} \quad (12)$$

Since the Hamiltonian is  $SU(N)$  symmetric, this operator transforms under  $SU(N)$  with the representation  $F \otimes F^* = id \oplus ad$ : the tensor product of the fundamental  $F$  (one box in the Young tableau language) and its complex conjugate  $F^*$  ( $N-1$  boxes), which reduces to the sum of the identity  $id$  and the adjoint  $ad$ . If we denote by  $R$  the ground state representation (a column

with  $Q = nN$  boxes), the tensor structure of  $J$  is then given by the Wigner-Eckart theorem: we have to find the occurrence of  $R$  in  $(id \oplus ad) \otimes R$ . We have a trivial term  $id \otimes R = R$  and a single non trivial one since  $ad \otimes R = R \oplus \dots$ , where  $\dots$  denotes other irreducible representations. Then we have :

$$\left\langle \nu \left| d_{\sigma} \frac{1}{H_H - E_{gs}} d_{\sigma'}^{\dagger} \right| \mu \right\rangle = A_1 \delta_{\sigma\sigma'} \delta_{\mu\nu} + B_1 C_{\mu\nu}^{\sigma\sigma'} \quad (13)$$

where  $C$  are the Clebsch-Gordan coefficients  $\langle R | ad \otimes R \rangle$ .

In order to avoid the computation of  $C$ , we can use the following argument. Let us consider the operator  $d_{\sigma} d_{\sigma'}^{\dagger}$ , which has the same symmetry as  $O_1$ , so the previous symmetry argument gives

$$\left\langle \nu \left| d_{\sigma} d_{\sigma'}^{\dagger} \right| \mu \right\rangle = A_2 \delta_{\sigma\sigma'} \delta_{\mu\nu} + B_2 C_{\mu\nu}^{\sigma\sigma'} \quad (14)$$

with the *same*  $C$ , but *different coefficients*  $A_2, B_2$ . Since  $B_2 \neq 0$ , we can eliminate  $C$  between the two equations. We finally obtain the general form, valid to first order in  $V_L^2$  for a  $SU(N)$  symmetric model:

$$J_{\mu\nu}^{\sigma\sigma'} = A \delta_{\sigma\sigma'} \delta_{\mu\nu} + B \left\langle \mu \left| d_{\sigma'}^{\dagger} d_{\sigma} \right| \nu \right\rangle \quad (15)$$

In this expression,  $A(N, n; V_H/U)$  and  $B(N, n; V_H/U)$  are dimensionless coefficients which depend only on the dimensionless ratio  $V_H/U$  associated with the high-energy problem (and of course a priori also on orbital number  $N$  and density  $n$ ).

Inserting (15) into equation (10), we obtain the simplified form of the conditions which determine the critical couplings:

$$\frac{U_{c1}^2}{t^2} = (A + nB)^2 + B^2 n(1-n)(N+1) \quad (16a)$$

$$\begin{aligned} \frac{U_{c2}^2}{t^2} &= (A + nB)^2 + B^2 n(1-n)(N+1) \\ &\quad - B^2 \sum_{\sigma\sigma'} \left\langle S_{\sigma\sigma'} c_{\sigma'}^{\dagger} c_{\sigma} \right\rangle \end{aligned} \quad (16b)$$

### C. The atomic limit

The atomic limit approximation is defined by  $V_H = 0$ . In this limit, the states  $|\mu\rangle$  are just the impurity states  $|\mu\rangle_0 \equiv |\sigma_1 \dots \sigma_Q\rangle$  ( $Q = 0, \dots, N$ ), without mixing with the high-energy electron sector. In that case,  $A$  and  $B$  (from (15)) can be computed explicitly (we choose here  $\tilde{\mu} = 0$ , i.e. the chemical potential is bound to be at the center of a step in the Coulomb staircase). We find:

$$A = -2, B = 4 \quad (17)$$

We note that these coefficients do not depend on  $N$  in the atomic limit. Moreover, it is clear that, in general (for an explicit proof, see Sec.IIID) :

$$\sum_{\sigma\sigma'} \left\langle S_{\sigma\sigma'} c_{\sigma'}^{\dagger} c_{\sigma} \right\rangle \propto N^2 \quad (18)$$

When using these results into (16a-16b), we obtain the  $N$ -dependence of the critical couplings quoted in (11a-11b).

This derivation relies on the use of the atomic limit  $V_H = 0$ . An important question is therefore to check that the  $N$ -dependence of the critical couplings is not modified by the interaction  $V_H$  that dresses the atomic states  $|\mu\rangle$ . We examine carefully this question in Appendix A, where we give an explicit proof that this is indeed the case. The problem is in fact quite different for  $U_{c1}$  and  $U_{c2}$ . For the latter,  $U$  must be scaled as  $U = N\tilde{U}$ . In that case, we show in the appendix that the atomic limit calculation of  $A$  and  $B$  is in fact *exact* at large  $N$ . This can be expected since the band gap diverges with  $N$ , so that the Hubbard bands are well separated from the low energy degrees of freedom. However, one might worry that the growing number of orbitals ( $N$ ) could counterbalance this effect. This is actually not the case, and we show that the corrections to  $J$  (or  $A, B$ ) coming from  $V_H$  are subdominant in large- $N$ , order by order in perturbation theory. Moreover, the low-energy effective Kondo problem becomes exactly solvable when  $U \propto N$  (i.e close to  $U_{c2}$ ): this is the subject of the next section (Sec. III D), in which the exact value of the prefactor  $\tilde{U}_{c2}$  is obtained.

The problem is more involved for  $U_{c1}$ , corresponding to the scaling  $U \propto \sqrt{N}$ . In that case, corrections in  $V_H$  beyond the atomic limit do produce corrections to  $A$  and  $B$  (hence to  $J$ ). However, we are able to show (Sec. A 2 of the appendix) that these corrections are of order one, so that the scaling  $U_{c1} = \sqrt{N}\tilde{U}_{c1}$  does hold.

#### D. Explicit large- $N$ solution of the effective low energy Kondo problem at $U_{c2}$

In this section, we explicitly solve the low energy effective Kondo problem in the large- $N$  limit using standard methods [26], in order to obtain the prefactor  $\tilde{U}_{c2}$ . The effective Hamiltonian (8) reduces at order  $(1/N^2)$  to:

$$H_{\text{eff}} = \sum_{k \in L, \sigma} \epsilon_k c_{k, \sigma}^\dagger c_{k, \sigma} + \frac{4V_L^2}{N\tilde{U}} \sum_{kk' \in L, \sigma\sigma'} \left( f_{\sigma'}^\dagger f_\sigma - \frac{\delta_{\sigma\sigma'}}{2} \right) c_{k, \sigma}^\dagger c_{k', \sigma'} \quad (19)$$

This model becomes exactly solvable at large  $N$  because the Kondo coupling scales as  $1/N$  (which is a result of  $U \propto N$ ). Introducing an auxiliary boson field  $b$  conjugate to  $\sum_{k\sigma} f_\sigma^\dagger c_{k\sigma}$ , and a Lagrange multiplier field  $\lambda$  to enforce the constraint  $\sum_{\sigma} f_\sigma^\dagger f_\sigma = Nn$ , we see that, as  $N \rightarrow \infty$ , the field  $b$  undergoes a Bose condensation, and the saddle-point values of the  $b, \lambda$  fields are determined

by the equations (at  $T = 0$ ):

$$G_f^{-1}(\omega) = \omega + \lambda - b^2 G_{cL}^0(\omega) \quad (20a)$$

$$n = -\frac{1}{\pi} \int_{-\infty}^0 d\omega \text{Im} G_f(\omega) \quad (20b)$$

$$\frac{\tilde{U}_{c2}}{4V_L^2} = \int d\tau G_f(\tau) G_{cL}^0(\tau) = \frac{1}{\pi} \int_{-\infty}^0 d\omega \text{Im}[G_f(\omega) G_{cL}^0(\omega)] \quad (20c)$$

In this expression,  $G_{cL}^0$  denotes the Green's function of the low-energy part of the effective bath of conduction electrons, in the absence of Kondo coupling, namely:

$$G_{cL}^0(i\omega) = \sum_{k \in L} \frac{1}{i\omega - \epsilon_k} = \frac{1}{V_L^2} \Delta_L(i\omega) \quad (21)$$

First we express the self-consistency condition (3) or more precisely its low-energy counterpart. We relate the low-energy part of the on-site Green's function,  $G_{dL}(i\omega_n)$ , to the auxiliary-fermion one,  $G_f(i\omega_n)$ , by imposing that the low-energy part of the interacting Green's function of the effective bath of conduction electrons,  $G_{cL}$ , can be calculated either from the original Anderson model or from the low-energy projected Kondo model, with identical results.  $G_{cL}$  is related to  $G_{cL}^0$  through the conduction electron  $\mathcal{T}$ -matrix:

$$G_{cL} = G_{cL}^0 + (G_{cL}^0)^2 \mathcal{T} \quad (22)$$

The Anderson model  $\mathcal{T}$ -matrix is  $V_L^2 G_{dL}$ , while it is  $b^2 G_f$  for the low-energy Kondo model. Therefore  $G_{dL}$  is directly related to  $G_f$  by:

$$V_L^2 G_{dL} = b^2 G_f \equiv \mathcal{T} \quad (23)$$

Using this into Eq.(20a), one finds the expression of  $G_{dL}$  in terms of the low-energy hybridization  $\Delta_L$ :

$$G_{dL}^{-1}(i\omega_n) = \frac{1}{Z} (i\omega_n + \lambda) - \Delta_L(i\omega_n) \quad (24)$$

where we have introduced the notation:

$$Z \equiv \frac{b^2}{V_L^2} \quad (25)$$

We can finally obtain  $G_{dL}$  in closed form by making use of (24) into the self-consistency condition (3) (restricted to the low-energy sector). This yields:

$$G_{dL}(i\omega) = \int d\varepsilon \frac{D(\varepsilon)}{\Delta_L(i\omega) + G_{dL}^{-1}(i\omega) - \varepsilon} \quad (26)$$

$$= \int d\varepsilon \frac{D(\varepsilon)}{\frac{1}{Z}(i\omega + \lambda) - \varepsilon} \quad (27)$$

The low-energy part of the local spectral density reads:

$$\rho_{dL}(\omega) \equiv -\frac{1}{\pi} \text{Im} G_{dL}(\omega + i0^+) = D\left(\frac{\omega + \lambda}{Z}\right) \quad (28)$$

By comparing this form of  $G_{dL}$  to its expression in terms of the local self-energy, we recognize that  $Z$  is the quasi-particle weight and  $\lambda$  yields the zero-frequency limit of  $\Sigma_d$ :

$$\mu - \Sigma_d(0) = \frac{\lambda}{Z}, \quad Z = \left[1 - \frac{\partial \Sigma_d}{\partial \omega} \Big|_{\omega=0}\right]^{-1} \quad (29)$$

The value of  $\lambda/Z$  can be determined by using the explicit form of  $\rho_d = Z\rho_f$  into (20b):

$$n = \int_{-\infty}^0 d\omega \frac{1}{Z} D\left(\frac{\omega + \lambda}{Z}\right) \quad (30)$$

Changing variables, this leads to  $\lambda/Z = \mu_0(n)$  where  $\mu_0(n)$  is the non-interacting value of the chemical potential, defined by:

$$n = \int_{-\infty}^{\mu_0} d\varepsilon D(\varepsilon) \quad (31)$$

We note that this is precisely the result expected from Luttinger's theorem (we have  $\mu - \Sigma_d(0) = \mu_0(n)$  which insures that the Fermi surface volume is unchanged by interactions). Hence, the low-energy part of the spectral function (quasi-particle resonance) is simply given by:

$$\rho_{dL}(\omega) = D\left(\frac{\omega}{Z} + \mu_0(n)\right) \quad (32)$$

Its shape is simply given by the non-interacting d.o.s., centered at  $\omega = -Z\mu_0$  and with a width renormalized by  $Z$ .

Second, we can now use (20c) and  $\text{Im}[\Delta_L G_f] = \frac{\omega + \lambda}{Z} \text{Im} G_f$ , to obtain :

$$\frac{\tilde{U}_{c2}}{4} = -\frac{1}{Z^2} \int_{-\infty}^0 d\omega (\omega + \lambda) \rho_{dL}(\omega) \quad (33)$$

$$= -\int_{-\infty}^0 \frac{d\omega}{Z} \frac{\omega + \lambda}{Z} D\left(\frac{\omega + \lambda}{Z}\right) \quad (34)$$

Clearly,  $Z$  drops out of this equation, which has therefore a unique solution, the critical coupling  $\tilde{U}_{c2}$  at which  $Z$  vanishes. This is expected: the low-energy effective Hamiltonian is valid only exactly at the critical point. A determination of the critical behaviour of  $Z$  slightly away from the critical point would require considering higher-order terms in the effective low-energy Hamiltonian. We therefore obtain the large- $N$  value of the critical coupling (using the expression of  $\lambda/Z$  found above):

$$\tilde{U}_{c2} = \frac{U_{c2}}{N} = 4\varepsilon_0(n) \quad (35)$$

with:

$$\varepsilon_0(n) \equiv -\int_{-\infty}^{\mu_0(n)} d\varepsilon \varepsilon D(\varepsilon) \quad (36)$$

This result is reminiscent of the critical coupling obtained in the Gutzwiller or slave-boson methods [24]: a detailed

comparison is made in Sec.IV. Taking for example a rectangular d.o.s. of half-width  $D$ , Eq.(35) yields:

$$\frac{U_{c2}}{N} = 4D n(1-n) \quad (37)$$

$\tilde{U}_{c2}$  is largest at half-filling ( $n = 1/2$ ). This is because orbital fluctuations are maximum there, so that it is more difficult to destroy the metallic phase (see however [18]). Obviously, for finite  $N$ , a Mott transition is found only for rational values of  $n = Q/N$  with integer  $Q$  (these values are dense on the interval  $[0, 1]$  as  $N$  becomes large).

Another way to obtain  $U_{c2}$  is to use the criterion of section III C together with the present large- $N$  limit in order to compute the matrix element  $\sum_{\sigma\sigma'} \langle S_{\sigma\sigma'} c_{\sigma'}^\dagger c_\sigma \rangle$ . This can be exactly evaluated at  $N = \infty$  using the effective action for the Kondo model (20):

$$\begin{aligned} S_{\text{eff}} = & \int_0^\beta d\tau \sum_\sigma f_\sigma^\dagger \partial_\tau f_\sigma - \lambda \sum_\sigma (f_\sigma^\dagger f_\sigma - n) \\ & + \int_0^\beta d\tau \frac{-N\tilde{U}}{4V_L^2} b^2 + \sum_\sigma b f_\sigma^\dagger c_\sigma + b c_\sigma^\dagger f_\sigma \\ & - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_\sigma^\dagger(\tau) G_{cL}^0(\tau - \tau')^{-1} c_\sigma(\tau') \end{aligned} \quad (38)$$

Because this action is gaussian, it is straightforward to get the following average (here  $\sigma \neq \sigma'$ ):

$$\begin{aligned} \langle f_\sigma^\dagger f_{\sigma'} c_{\sigma'}^\dagger c_\sigma \rangle = & \left\langle f_\sigma^\dagger f_{\sigma'} \int_0^\beta d\tau G_{cL}^0(\tau) b f_{\sigma'}^\dagger(\tau) \int_0^\beta d\tau' G_{cL}^0(\tau') b f_\sigma(\tau') \right\rangle \\ = & -b^2 \left[ \int_0^\beta d\tau G_{cL}^0(\tau) G_f(\tau) \right]^2 \end{aligned} \quad (39)$$

We find therefore:

$$\sum_{\sigma\sigma'} \langle S_{\sigma\sigma'} c_{\sigma'}^\dagger c_\sigma \rangle = -N^2 b^2 \left[ \int d\tau G_f(\tau) G_{cL}^0(\tau) \right]^2 + \mathcal{O}(N) \quad (40)$$

which indeed scales as  $N^2$ . Inserting this into (16b), we have :

$$U_{c2} = 4t \frac{V_L}{\sqrt{Z}t} N b \int d\tau G_f(\tau) G_{cL}^0(\tau) \quad (41)$$

which coincides with Eq. (20c) since  $\sqrt{Z} = b/V_L$ . Hence, we have checked that both methods (explicit large- $N$  solution and projective criterion of Sec.III C) yield the same result for the critical interaction  $U_{c2}$ .

#### IV. COMPARISON TO A SLAVE-BOSON APPROACH

In this section, we show that a multiorbital slave boson approximation reproduces the previous results close

to the critical coupling  $U_{c2}$ . This method is an extension to many orbitals of the Gutzwiller approximation, formulated in terms of slave bosons by Kotliar and Ruckenstein [27] and extended to many orbitals in [28]. Indeed, with the scaling  $U = N\tilde{U}$ , the Mott gap is of order  $N$  and quasiparticles dominate the physics over most of the energy range. Furthermore, the expression (28) for the physical spectral function close to  $U_{c2}$  contains precisely the same ingredients than in slave boson methods, namely: a shift of the effective level which insures Luttinger's theorem, and a quasiparticle weight  $Z$  (vanishing at the transition). The self-energy contains no further renormalizations (in particular the quasi-particle lifetime is infinite). This bare-bone picture of a strongly correlated Fermi liquid is precisely that emphasized by slave boson approaches.

Following [28], one introduces  $2^N$  slave bosons  $\phi_{\sigma_1 \dots \sigma_p}$  associated with a given spin configuration  $\sigma_1 \dots \sigma_p$  on the impurity orbital. The probability that the orbital is in a given spin configuration is simply given by  $\langle \phi_{\sigma_1 \dots \sigma_p}^\dagger \phi_{\sigma_1 \dots \sigma_p} \rangle$ . The physical electron operator is represented as:

$$d_\alpha^\dagger = z_\alpha f_\alpha^\dagger \quad (42)$$

with:

$$\begin{aligned} z_\alpha &\equiv g_1 \left( \sum_p \sum_{\alpha \notin (\sigma_1, \dots, \sigma_p)} \phi_{\sigma_1 \dots \sigma_p}^\dagger \phi_{\sigma_1 \dots \sigma_p} \right) g_2 \quad (43) \\ g_1 &\equiv \left[ 1 - \sum_p \sum_{\alpha \in (\sigma_1, \dots, \sigma_p)} \phi_{\sigma_1 \dots \sigma_p}^\dagger \phi_{\sigma_1 \dots \sigma_p} \right]^{-1/2} \\ g_2 &\equiv \left[ 1 - \sum_p \sum_{\alpha \notin (\sigma_1, \dots, \sigma_p)} \phi_{\sigma_1 \dots \sigma_p}^\dagger \phi_{\sigma_1 \dots \sigma_p} \right]^{-1/2} \end{aligned}$$

This representation is supplemented by two constraints:

$$f_\alpha^\dagger f_\alpha = \sum_p \sum_{\alpha \in (\sigma_1, \dots, \sigma_p)} \phi_{\sigma_1 \dots \sigma_p}^\dagger \phi_{\sigma_1 \dots \sigma_p} \quad (44a)$$

$$1 = \sum_p \sum_{(\sigma_1 \dots \sigma_p)} \phi_{\sigma_1 \dots \sigma_p}^\dagger \phi_{\sigma_1 \dots \sigma_p} \quad (44b)$$

At this stage, this is an exact representation of the Hilbert space, which can be used to rewrite the Hubbard Hamiltonian. In order to obtain an approximate solution, we shall assume that all auxiliary bosons undergo a Bose-condensation, i.e become static c-numbers, and that furthermore the corresponding expectation value depends only on the total charge  $p$  and not on the specific spin configuration  $\sigma_1, \dots, \sigma_p$ . We shall thus set, at each site:

$$\phi_{i\sigma_1 \dots \sigma_p} = \phi_p \quad (45)$$

We emphasize that this approximation *does not* correspond to a controlled saddle-point, even in the large- $N$

limit, since the number of auxiliary fields grows rapidly with  $N$ .

Using this Ansatz, the Hubbard Hamiltonian can be rewritten in the form:

$$H = - \sum_{i,j} \sum_{\sigma=1}^N t_{ij} z^2 f_{i\sigma}^\dagger f_{j\sigma} + \frac{U}{2} \sum_i \sum_{p=0}^N \binom{N}{p} \phi_p^2 (p - Nn)^2 \quad (46)$$

with:

$$z = \frac{1}{\sqrt{n(1-n)}} \sum_{p=0}^{N-1} \binom{N-1}{p} \phi_p \phi_{p+1} \quad (47)$$

and the constraints:

$$\sum_{p=0}^N \binom{N}{p} \phi_p^2 = 1 \quad (48)$$

$$\sum_{p=1}^N \binom{N-1}{p-1} \phi_p^2 = n \equiv \langle f_\sigma^\dagger f_\sigma \rangle \quad (49)$$

The free-energy corresponding to this Hamiltonian must then be minimized with respect to the  $N+1$  variational parameters  $\phi_p$ 's, subject to the two constraints above. In the following, we briefly outline this procedure, focusing for simplicity on the half-filled case ( $n = 1/2$ ) at zero-temperature.

In this case, particle-hole symmetry makes the analysis simpler. It implies that  $\phi_p = \phi_{N-p}$ , and it can then be shown that the constraint  $\sum_{p=1}^N \binom{N-1}{p-1} \phi_p^2 = n = 1/2$  is automatically satisfied when the first one ( $\sum_{p=0}^N \binom{N}{p} \phi_p^2 = 1$ ) is. Evaluating the ground-state energy of (46) yields the following expression to be minimized at  $T = 0$  (subject to just one constraint):

$$\begin{aligned} \frac{1}{N} E_0 &= -4\varepsilon_0 \left[ \sum_{p=0}^{N-1} \binom{N-1}{p} \phi_p \phi_{p+1} \right]^2 \\ &+ \frac{\tilde{U}}{2} \sum_{p=0}^N \binom{N}{p} \phi_p^2 \left( \frac{N}{2} - p \right)^2 \quad (50) \end{aligned}$$

with  $\varepsilon_0$  the (absolute value) of the non-interacting kinetic energy per orbital (as defined in (36)), and  $\tilde{U} \equiv U/N$ , as defined above.

It is clear from the Hamiltonian (46) that this slave-boson approximation leads to a picture of quasiparticles with no residual interactions. The quasiparticle weight reads:

$$Z = z^2 = \frac{1}{n(1-n)} \left( \sum_{p=0}^{N-1} \binom{N-1}{p} \phi_p \phi_{p+1} \right)^2 \quad (51)$$

while the chemical potential shift  $\lambda$  in the previous section corresponds in the present context to the Lagrange

multiplier associated with the constraint (44a) (it vanishes at half-filling).

We also note that the non-interacting limit is correctly reproduced, thanks to the square-root normalization factors [27] introduced in (43). In that limit,  $Z = 1$  and  $E_0 = -N\varepsilon_0$ .

In order to analyze the Mott transition, we note that within this approach, an insulating solution can be found *for arbitrary strength of the coupling  $U$* . It corresponds to the trivial solution:

$$\phi_{N/2}^2 = \left(\frac{N}{N/2}\right)^{-1}, \quad \phi_p = 0 \quad (p \neq \frac{N}{2}) \quad (52)$$

which yields the  $T = 0$  occupancies in the atomic limit. This solution is always an extremum of the variational energy (corresponding to a boundary), but not always a *minimum*. Indeed, a minimum with a lower energy exists for  $\tilde{U} < \tilde{U}_{c2}$ . To find this critical coupling, we perturb around the trivial solution. Close to  $U_{c2}$ , only the occupancies of the states with charge  $N/2 \pm 1$  matter, and we set:  $\phi_{N/2}^2 = \left(\frac{N}{N/2}\right)^{-1} + \dots$ ,  $\phi_{N/2 \pm 1} = \delta\phi$ , and  $\phi_p = \dots$  otherwise (where  $(\dots)$  denote terms that can be neglected). The energy difference with the trivial insulating solution reads:

$$\begin{aligned} \Delta E = & -4\varepsilon_0 \frac{\left(\left(\frac{N-1}{N/2}\right) + \left(\frac{N-1}{N/2-1}\right)\right)^2}{\left(\frac{N}{N/2}\right)} \delta\phi^2 \\ & + \frac{\tilde{U}}{2} \left( \left(\frac{N}{N/2-1}\right) + \left(\frac{N}{N/2+1}\right) \right) \delta\phi^2 \end{aligned} \quad (53)$$

Hence, the critical coupling at which the metallic solution disappears reads:

$$\tilde{U}_{c2} = 16\varepsilon_0 \frac{\left(\frac{N-1}{N/2}\right)^2}{\left(\frac{N}{N/2}\right)\left(\frac{N}{N/2-1}\right)} = 4\varepsilon_0 \frac{N+2}{N} \quad (54)$$

This value coincides with that obtained by Lu [24] using the Gutzwiller approximation. Remarkably, it agrees with our exact result in the  $N \rightarrow \infty$  limit. Together with the considerations above, this suggests that such a slave boson approach becomes asymptotically exact, at low-energy and close to the critical coupling  $U_{c2}$ , in this limit. This estimate of the critical coupling is already quite accurate for the smallest value of  $N = 2$  (we take for reference a semi-circular band with half-width  $D = 1$ ):

$$U_c(N=2) = \frac{8D}{3\pi}(N+2) \simeq 3.3 \quad (55)$$

(the NRG and the projective analysis of the one-orbital model indicate that  $U_c$  is very close to 3). On the other hand, the large- $N$  solution given by equation (35) misses obviously the sub-leading term of order  $N^0$ , and is therefore inaccurate at small  $N$ .

The behaviour of the quasi-particle weight close to the transition can be obtained by expanding the energy to next order in  $\delta\phi$ , taking into account that  $\phi_{N/2 \pm q}^2 \sim (1 - \tilde{U}/\tilde{U}_{c2})^q$  (so that only the terms with  $q = 0, \pm 1$  matter). This yields:

$$Z = 1 - \frac{U}{U_{c2}} + \dots \quad (56)$$

We note that there are no  $1/N$  prefactors in this expression when couplings are scaled properly.

It is not entirely obvious to decide what the critical coupling  $U_{c1}$  is within this approach. Since the insulating solution exists for arbitrary  $U$ , one might be tempted to conclude that  $U_{c1} = 0$ . Another criterion would be to find at which coupling the optical gap of the insulator vanishes. Unfortunately, the above approximation (condensed bosons) is insufficient to discuss high-energy features (Hubbard bands). Studies that go beyond this approximation [29] and incorporate fluctuations of the slave bosons suggest that the optical gap closes at  $U_{c2}$ : in that sense the slave boson approximation does not yield a coexistence regime, in contrast to the exact results established above (which are the generic situation within DMFT).

## V. FINITE TEMPERATURE TRANSITIONS

We conclude this paper by addressing the finite-temperature aspects of the transitions discussed above. As in the one-band case, we expect a coexistence region  $U_{c1}(T) \leq U \leq U_{c2}(T)$  at finite temperature, which closes at a second-order (liquid-gas) critical point  $(U_{\text{MIT}}, T_{\text{MIT}})$ , with  $U_{c1}(T_{\text{MIT}}) = U_{c2}(T_{\text{MIT}}) = U_{\text{MIT}}$ . Comparison of free-energies then yield a first-order transition line  $T = T_c(U)$  for  $T < T_{\text{MIT}}$ . This has been the subject of many studies in the single orbital case, and is now established on firm grounds. However, no analytical estimate of the critical temperature  $T_{\text{MIT}}$  is available. This is highly desirable, since this scale appears to be strongly reduced in comparison to the electronic bandwidth. It would also be interesting to know how this scale depends on the orbital degeneracy.

Let us start with a qualitative argument, which has two merits in our view: (i) it allows to understand why  $T_{\text{MIT}}/t$  is such a small energy scale for a small number of orbitals and (ii) it provides a *lower* bound on  $T_{\text{MIT}}$ . This argument is based on a comparison of the energy difference between the metallic and insulating solutions at  $T = 0$ , to the corresponding entropy difference. For  $U = N\tilde{U}$  close to  $U_{c2}$ , the energy difference  $\Delta E_0 \equiv E_I(T=0) - E_M(T=0)$  is expected to behave as:

$$\Delta E_0 = N \frac{(\tilde{U}_{c2} - \tilde{U})^2}{\tilde{U}_{c2}} + \dots \quad (57)$$



This is indeed supported by the slave-boson calculation of Sec.IV. The entropy difference  $\Delta S = S_I - S_M$  is dominated by the entropy of the insulating solution (which has a degenerate ground-state) since the entropy of the metal vanishes linearly with  $T$  at low temperature  $T$ . Therefore:

$$\Delta S_0 \sim \ln \left( \frac{N}{N/2} \right) \sim N \ln 2 \quad (58)$$

This allows to estimate the behaviour of the first-order critical line  $U_c(T)$  (or  $T_c(U)$ ) at low-temperature (i.e for  $U$  close to  $U_{c2}$ ). Indeed, the transition into the insulating state upon raising temperature occurs when the entropic gain overcomes the energy cost, leading to:

$$T_c(U) \simeq \frac{(\tilde{U}_{c2} - \tilde{U})^2}{\tilde{U}_{c2}} \quad (59)$$

This estimate is valid only at very low temperature, close to the  $T = 0$  critical point  $U = U_{c2}$ . It indicates a quadratic dependence of the critical line, with a prefactor which is independent of  $N$  [30].

When  $U_{c1}$  is close to  $U_{c2}$ , which is the case for a small number of orbitals (in particular in the one-band case), one can roughly estimate the critical endpoint  $T_{\text{MIT}}$  by using (59) in the regime of couplings where the insulating solution disappears, leading to:  $T_{\text{MIT}} \simeq (\tilde{U}_{c2} - U_{c1}/N)^2 / \tilde{U}_{c2}$ . It is clear from this formula that the ratio  $T_{\text{MIT}}/t$  is small because of the small energy difference between the metallic and insulating solutions. For a larger number of orbitals however, this can only produce a *lower bound* on the critical endpoint  $T_{\text{MIT}}$ . Indeed, the energy difference close to  $T_{\text{MIT}}$  is certainly underestimated by (57), while the entropy difference is reduced as compared to  $N \ln 2$  since the entropy of the metal cannot be neglected at  $T_{\text{MIT}}$  (we note that it behaves as  $\gamma T$  with  $\gamma \propto N$ ). This argument shows that  $T_{\text{MIT}}/t$  must either saturate to a constant, or increase with  $N$ , as  $N$  increases.

We now turn to a more quantitative study of these finite-temperature issues, using the Landau functional formalism introduced in [14]. A functional of the effective hybridisation is introduced, which reads, for the  $N$ -orbital model on the Bethe lattice (semi-circular d.o.s):

$$F[\Delta] = \frac{N}{2t^2} \frac{1}{\beta} \sum_n \Delta(i\omega_n)^2 + \ln Z_{\text{imp}}[\Delta] \quad (60)$$

in which  $Z_{\text{imp}}$  is the partition function  $Z = \text{Tr } e^{-S_{\text{imp}}}$  of the effective impurity model, defined by the action:

$$S_{\text{imp}} = \int_0^\beta d\tau \sum_\sigma d_\sigma^\dagger \partial_\tau d_\sigma + \frac{U}{2} \left[ \sum_\sigma (d_\sigma^\dagger d_\sigma - n) \right]^2 + \int_0^\beta d\tau \int_0^\beta d\tau' \Delta(\tau - \tau') \sum_\sigma d_\sigma^\dagger(\tau) d_\sigma(\tau') \quad (61)$$

This functional is locally stationary for these hybridisation functions which satisfy the DMFT equations:

$$\frac{\delta F}{\delta \Delta} = 0 \Leftrightarrow \Delta(i\omega_n) = t^2 G(i\omega_n) \quad (62)$$

The local stability of these DMFT solutions is controlled by the matrix of second derivatives:

$$\chi_{nm} \equiv \frac{\delta^2 F}{\delta \Delta(i\omega_n) \delta \Delta(i\omega_m)} = \frac{N}{t^2} + K_{nm} \quad (63)$$

with, using (60,61):

$$K_{nm} = \frac{1}{\beta^2} \int_0^\beta \cdots \int_0^\beta d\tau_1 d\tau'_1 d\tau_2 d\tau'_2 e^{i\omega_n(\tau'_1 - \tau_1) + i\omega_m(\tau'_2 - \tau_2)} \sum_{\sigma_1 \sigma_2} [\langle T_\tau d_{\sigma_1}^+(\tau_1) d_{\sigma_1}(\tau'_1) d_{\sigma_2}^+(\tau_2) d_{\sigma_2}(\tau'_2) \rangle - \langle T_\tau d_{\sigma_1}^+(\tau_1) d_{\sigma_1}(\tau'_1) \rangle \langle T_\tau d_{\sigma_2}^+(\tau_2) d_{\sigma_2}(\tau'_2) \rangle] \quad (64)$$

A solution of the DMFT equations is locally stable provided the  $\chi_{nm}$  matrix has no negative eigenvalues when evaluated for this solution. Hence, the couplings  $U_{c1}(T)$  (resp.  $U_{c2}(T)$ ) correspond to the instability line of the  $(U, T)$  plane along which a negative eigenvalue appears when  $\chi_{nm}$  is evaluated for the insulating (resp. metallic) solution. For  $T = 0$ , these instability criteria should coincide with those derived from the projective method described above (as verified below for  $U_{c1}(T = 0)$ ). The critical endpoint  $T = T_{\text{MIT}}$  is such that, for  $T > T_{\text{MIT}}$ , no negative eigenvalue is found, at any coupling  $U$ , when the stability matrix is evaluated on the (unique) DMFT solution. It should thus be noted that, in order to determine  $(U_{\text{MIT}}, T_{\text{MIT}})$ , it is not necessary to know *both*  $U_{c1}(T)$  and  $U_{c2}(T)$ : either one of them is in principle sufficient.

The practical difficulty in performing this stability analysis at finite temperature is that: (i) it requires a knowledge of the finite- $T$  solution of the DMFT equations -or at least a reasonable approximation to it- and (ii) the two-particle correlator (64) must be evaluated for this solution. Completing this program, for arbitrary orbital degeneracy, using numerical methods, is beyond the scope of this paper. However, we would like to present here a simpler calculation which gives some insight in the dependence of  $U_{c1}(T)$  (and of  $T_{\text{MIT}}$ ) on the orbital degeneracy  $N$ . What we have done is to use the atomic limit as a very rough first approximation to the insulating solution. We have evaluated the 2-particle correlator  $K_{nm}$  and the stability matrix  $\chi_{nm}$  in this limit, for arbitrary  $N$ . This can be directly implemented on the computer, using the spectral decomposition of  $K_{nm}$  onto atomic eigenstates (some details are provided in Appendix B). The stability matrix is then diagonalised numerically (a truncation to a -large- number of Matsubara frequencies is made), and we search for the line in the  $(U, T)$  plane where a negative eigenvalue is first found.

The result of this calculation (for the half-filled case  $n = 1/2$ ) is depicted in Fig. 1. There, the temperature below which a negative eigenvalue is found is plotted as a function of  $U$ . We first observe that no instability is

found above a critical value of  $U$ , which does coincide with the value (16a):  $U_{c1}(T=0)/t \simeq 4\sqrt{N+1}$  estimated above from the projective method (in the atomic approximation). This is a non-trivial consistency check on our calculations. Secondly, we find that the instability lines for different values of the orbital degeneracy  $N$  can all be collapsed on a single curve when both  $T$  and  $U$  are rescaled by  $\sqrt{N+1}$ . This can be understood from the fact that, in the atomic limit, only the two scales  $U$  and  $T$  enter the two-particle correlator  $K_{nm}$  (*not*  $t$ ), and that  $K$  is of order  $N^2$ , so that the instability criterion can be written (from dimensionality considerations):  $\frac{\tilde{U}}{t} = \Phi(\frac{T/\sqrt{N+1}}{U})$ . Naturally, we do not expect the curve in Fig. 1 to be a quantitatively reliable determination of  $U_{c1}(T)$ , because of the atomic approximation involved. In particular, we see that, instead of terminating at a critical endpoint ( $U_{\text{MIT}}, T_{\text{MIT}}$ ), the instability line in Fig. 1 bends back, yielding a stability window at small  $U$  which is certainly a spurious aspect of the approximation. Hence only the branch of the curve corresponding to larger values of  $U$  has physical significance.

It is tempting to conclude, from the the observed scaling with  $\sqrt{N+1}$ , that  $T_{\text{MIT}}$  itself will grow in that manner as  $N$  is increased. Indeed, we note that recent QMC calculations by Amadon and Biermann [22] do show a marked increase of  $T_{\text{MIT}}$  with  $N$ , not inconsistent with a  $\sqrt{N}$  scaling. However, we do not consider this issue to be entirely settled: rather, this atomic estimate provides an *upper bound* on the growth of  $T_{\text{MIT}}$  with  $N$ . Indeed, it neglects the presence of the quasiparticle resonance (which is reduced but still present as temperature is raised close to  $T_{\text{MIT}}$ ). The resonance makes the solution less stable, so that the atomic calculation is likely to overestimate  $T_{\text{MIT}}$ . Combined with the above entropy argument (which provides a lower bound), we conclude that  $T_{\text{MIT}}/t$  is an increasing function of  $N$  at moderate values of  $N$ , which either saturates at large- $N$  or increases at most as  $\sqrt{N}$ . Clearly, a more refined analysis of the above stability condition is required to settle this issue.

## VI. CONCLUSION

In this paper, we have studied the Mott transition of the  $N$ -orbital Hubbard model in the fully symmetric case. The physical picture is qualitatively the same as for  $N=2$ , *i.e.* a coexistence region exists between an insulating and a metallic solution within two distinct critical couplings  $U_{c1}$  and  $U_{c2}$ . We have shown that these critical couplings *do not have the same dependence on the number of orbitals*, as the latter becomes large:  $U_{c1} \propto \sqrt{N}$  while  $U_{c2} \propto N$ . We have obtained an exact analytical determination of the critical value  $\tilde{U}_{c2} = U_{c2}/N$  in this limit. These results explain the widening of the coexistence window  $[U_{c1}, U_{c2}]$  observed in the numerical simulations of Ref. [21], and more recently in [22]. Our findings also put the results of Refs. [19, 20] in a new perspective, as discussed in the introduction.

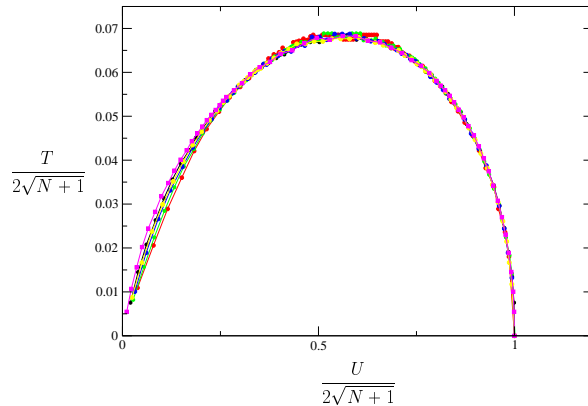


FIG. 1: Instability temperature below which a negative eigenvalue is found when the stability matrix  $\chi_{nm}$  of Eq. (63) is evaluated in the atomic approximation. The various curves are for increasing number of orbitals ( $N = 2, 4, 6, 8, 10, 20$ ), and an almost perfect scaling with  $T/\sqrt{N+1}$  and  $U/\sqrt{N+1}$  is found.

We have shown that, at large  $N$  and close to the critical coupling  $U_{c2}$ , the scaling  $U = N\tilde{U}$  is appropriate, so that the separation of scale which is at the heart of the projective method becomes asymptotically exact. The low-energy physics close to  $U_{c2}$  is then well described by slave-boson like approximations. This is the case in particular for the quasi-particle peak in the spectral function, which is separated from Hubbard bands by a large energy (of order  $N\tilde{U}$ ) and is accurately described by the simple form (32). In view of practical applications to electronic structure calculations with large orbital degeneracy (e.g f-electron systems), it would be highly desirable to have also an analytical determination of the high-energy part of the spectral function in the large- $N$  limit (or at least reasonable approximations to it). This is left for future investigations.

Another issue that we have only partly addressed is the finite-temperature aspects of these transitions. The whole finite-temperature coexistence region widens as  $N$  is increased, and the critical temperature associated with the Mott critical endpoint does increase with the number of orbitals at intermediate values of  $N$ . The precise behaviour of  $T_{\text{MIT}}/t$  at large  $N$  deserves further studies however.

## Acknowledgments

We thank B. Amadon and S. Biermann for useful discussions, and for sharing with us their recent QMC numerical results for this model. This work was supported by the NSF under grant NSF DMR 0096462 and by the PICS program of the CNRS (under contract PICS 1062).

## APPENDIX A: LARGE- $N$ SCALINGS AND THE ATOMIC LIMIT

In this appendix, we provide a detailed proof that the corrections in  $V_H$  to the atomic limit ( $V_H = 0$ ) do not modify the large- $N$  dependence of the critical couplings. This is done by an explicit investigation of the structure of these corrections. Moreover, we show that for  $U \propto N$  (i.e when  $U_{c2}$  is considered), these corrections only produce subdominant terms which can be ignored at large- $N$ .

### 1. Corrections in $V_H$ for $U = N\tilde{U}$ .

For our purpose, the operator  $H_H$  can be written :

$$\begin{aligned} H_H &= H_H^0 + H_H^1 \\ H_H^0 &= \sum_{k \in H^\pm, \sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \frac{U}{2} \left[ \sum_{\sigma} (d_{\sigma}^\dagger d_{\sigma} - n) \right]^2 \\ H_H^1 &= V_H \sum_{\sigma} \sum_k c_{k,\sigma}^\dagger d_{\sigma} + d_{\sigma}^\dagger c_{k,\sigma} \end{aligned} \quad (A1)$$

First let us consider the ground state energy  $E_{gs}$ . As the lower Hubbard band  $H^-$  is filled in  $|\mu\rangle_0$ , we prefer to remove the constant contribution  $\sum_{k \in H^-, \sigma} \epsilon_k$ , so that the zeroth order energy is  $E_0 = {}_0\langle \mu | H_H^0 | \mu \rangle_0 = 0$ . The next order term  $\delta E_1 = {}_0\langle \mu | H_H^1 | \mu \rangle_0$  is zero by conservation of the total charge  $Q$  on the  $d$ -level, so we need to look at the second order contribution:

$$\begin{aligned} \delta E_2 &= \sum_{|\psi\rangle} \frac{|\langle \psi | H_H^1 | \mu \rangle_0|^2}{E_0 - E_{\psi}} \\ &= -(N - Q) \sum_{k \in H^-} \frac{V_H^2}{\frac{U}{2} - \epsilon_k} - Q \sum_{k \in H^+} \frac{V_H^2}{\frac{U}{2} + \epsilon_k} \end{aligned} \quad (A2)$$

since  $|\psi\rangle$  can only possess a charge  $Q + 1$  (resp.  $Q - 1$ ) for the  $d$ -electron and a hole (resp. particle) excitation in the bath. Clearly as  $\epsilon_k$  is negative (positive) for  $k \in H^-$  ( $H^+$ ), the denominators are of order  $N$  (since  $U = N\tilde{U}$ ) and  $\delta E_2$  is therefore scaling as  $N^0$  at large  $N$ . We would like to infer this to be true at all order in the development in  $V_H$ . One can easily classify into two categories the intermediate states that appear at order  $V_H^4$  and beyond. There can either be a charge different from  $Q$  on the impurity (as in the previous computation at order  $V_H^2$ ) and then the denominator coming from this state provides (at least) a factor  $N^{-1}$  by the presence of the Coulomb energy  $U = N\tilde{U}$ . Or the impurity can be found in a charge  $Q$  state (with possibly a reorganization of the spin configuration) without a Coulomb energy cost. However this state possesses also many particle-hole excitations in the bath, and this leads to a denominator which scales as the Mott gap  $\Delta_g$ . For example let us consider such a ket generated at order  $V_H^4$ , like

$|\sigma_1 \dots \sigma_Q\rangle_d |2 \dots N\rangle_- |1\rangle_+$ . This particular state (but the argument is general), contributes a factor  $(\epsilon_k - \epsilon_{k'})^{-1}$  where  $k \in H^-$  and  $k' \in H^+$ . This quantity is always smaller than  $\Delta_g^{-1}$  because the Mott gap  $\Delta_g$  is also the gap of the  $c_{k,\sigma}$  electrons (through the self-consistency). As the gap  $\Delta_g$  is expected to be of order  $U = N\tilde{U}$  when  $U$  is close to  $U_{c2}$ , each particle-hole excitation also provides a factor  $N^{-1}$  in the perturbative expansion. This is enough to conclude that, at a given order in perturbation theory, each of the denominator gives a factor  $N^{-1}$  that balance the combinatorial factor coming from the string of charge excitation on the impurity level. Thus  $E_{gs}$  is at most of order 1 when  $N$  is large.

We finally need to compute  $J_{\mu\nu}^{\sigma\sigma'}$  at large  $N$ . Let us consider first the case  $\mu \neq \nu$ , so that  $\mu$  and  $\nu$  will differ by only one spin flip  $\sigma \leftrightarrow \sigma'$ . We can now calculate at the lowest order in  $V_H$  the desired matrix element:

$$\Gamma \equiv \langle \mu | d_{\sigma} \frac{1}{H_H^0 + H_H^1 - E_{gs}} d_{\sigma'}^\dagger | \nu \rangle \quad (A3)$$

with

$$\begin{aligned} |\mu\rangle &\equiv |\mu\rangle_0 + |\mu\rangle_1 \\ |\mu\rangle_1 &= \sum_{k \in H^-, \sigma} \frac{V_H}{\frac{U}{2} - \epsilon_k} d_{\sigma}^\dagger c_{k,\sigma} |\mu\rangle_0 + \sum_{k \in H^+, \sigma} \frac{V_H}{\frac{U}{2} + \epsilon_k} c_{k,\sigma}^\dagger d_{\sigma} |\mu\rangle_0 \end{aligned} \quad (A4)$$

The contribution at order  $(V_H)^0$  is therefore:

$$\delta \Gamma_0 = {}_0\langle \mu | d_{\sigma} \frac{1}{H_H^0 - E_{gs}} d_{\sigma'}^\dagger | \nu \rangle_0 \sim \frac{2}{U} \quad (A5)$$

because  $E_{gs} = \mathcal{O}(1)$  and  $U = N\tilde{U}$ . All terms coming at order  $V_H$  cancel by conservation of the charge, so we examine now the next leading order for  $\Gamma$ ,  $\delta \Gamma_2$ , which is composed of three terms: one from the correction by  $V_H$  to each of the two external kets, one from the development of the denominator in (A5) at order  $V_H^2$ , and a mixed term (between only one ket correction and the denominator developed at first order). Let us examine the first of these second order contributions:

$$\delta \Gamma_2^{(1)} = {}_1\langle \mu | d_{\sigma} \frac{1}{H_H^0 - E_{gs}} d_{\sigma'}^\dagger | \nu \rangle_1 \quad (A6)$$

The state  $d_{\sigma'}^\dagger |\nu\rangle_1$  is composed of charge  $Q + 2$  excitations (with energy  $2^2 U/2$ ) and of particle-hole excitations in the bath with a charge  $Q$  on the impurity (this has the energy  $\epsilon_k - \epsilon_{k'}$ ). Both energies scale like  $N$  and contribute an overall factor  $N^{-3}$  to  $\delta \Gamma_2^{(1)}$ . There is also a combinatorial factor of order  $N$  coming from the choice in the spin-excitation in  $|\nu\rangle_1$ , but there is none from the state  $|\mu\rangle_1$  as the spin configuration in  $d_{\sigma'}^\dagger |\mu\rangle_1$  is fixed by the one in  $d_{\sigma'} |\nu\rangle_1$ . Therefore  $\delta \Gamma_2^{(1)} = \mathcal{O}(N^{-2})$ . The same argument works for the two other contribution at order  $V_H^2$ .

More generally, at a given order  $p$  in the development in  $V_H$ , each of the  $p + 1$  denominators provides a factor of

order  $N^{-1}$ , because there is a finite gap  $\Delta_g \sim U_{c2} \propto N$  between the two Hubbard bands [25]. However the string of  $p$  spin-flips generated by the  $H_{\text{mix}}$  terms only contributes to an overall combinatorial factor at most  $N^{p/2}$  because one has to connect two fixed external configurations  $|\nu\rangle$  and  $|\mu\rangle$ . Hence in the limit of large  $N$  all terms after the first one are sub-dominant, so that:

$$\Gamma = \delta\Gamma_0 + \mathcal{O}\left(\frac{1}{N^2}\right) = \frac{2}{U} = \frac{2}{N\tilde{U}} \quad (\text{A7})$$

meaning that the atomic result for  $\Gamma$  is exact in the large- $N$  limit when  $U \propto N$ .

At this stage, we want to stress *a posteriori* that the hypotheses made in the preceding argument are consistent with this result. First it is correct to fix the chemical potential  $\tilde{\mu} = 0$  from the atomic limit ( $V_H = 0$ ), because perturbative corrections do not change the occupancy of the  $d$ -orbital, as can be checked from a direct expansion in  $V_H$  of  $\langle \sum_{\sigma} d_{\sigma}^{\dagger} d_{\sigma} \rangle$ . Finally the existence of a large Mott gap  $\Delta_g \propto N$  can also be justified on the same grounds.

## 2. Some remarks about $U_{c1}$

When  $U \propto \sqrt{N}$  on the other hand, the perturbative series for  $\Gamma$  does not appear to stop after the first contribution, showing that  $U_{c1}$  is affected by  $V_H$  in the large  $N$  limit. It is however straightforward to follow the line of arguments given in Section III C to see that each term in

this development provides a leading contribution of order  $1/\sqrt{N}$  ( using  $U \sim \Delta_g \propto \sqrt{N}$ ).  $\Gamma$  can not be computed exactly in that case, because  $B(N, n; V_H/(\sqrt{N}\tilde{U}))$  is now a non trivial function of  $V_H/\tilde{U}$  at  $N = \infty$ . But this is enough to conclude that  $B(N, n; V_H/U)$  is of order 1 at large  $N$  when  $U \propto \sqrt{N}$ , so that the result  $U_{c1} \sim \sqrt{N}\tilde{U}_{c1}$  holds. However, an exact evaluation of  $\tilde{U}_{c1}$  appears to be a difficult task, even at  $N = \infty$ .

## APPENDIX B: NUMERICAL CALCULATION OF THE STABILITY MATRIX IN THE ATOMIC LIMIT

In this Appendix, we provide details on the computation of the stability matrix  $\chi_{nm}$  in the  $N$ -orbital atomic limit (cf. Fig. 1). First, we use a spectral decomposition over the atomic eigenstates in Eq. (64). This yields:

$$K_{nm} = A(i\omega_n, -i\omega_n, i\nu_n, -i\nu_n)/Z_{at} - B(i\omega_n)B(i\nu_n)/Z_{at}^2$$

with

$$Z_{at} = \sum_{Q=0}^N e^{-\beta E_Q} \binom{N}{Q}$$

$$A(\omega_j, j = 1..4) \equiv N \sum_{\substack{0 \leq Q \leq N \\ P \in \mathcal{S}_4}} e^{-\beta E_Q} \epsilon(P) \left( C_1(Q, P) + (N-1)C_2(Q, P) \right) F_4(\omega_{P(j)} + \Delta_{Q+\sum_{i=j+1}^4 a_{P(i)}, a_{P(j)}}, j = 1..4)$$

$$B(i\omega_n) \equiv N \sum_{Q=0}^N e^{-\beta E_Q} \left[ \binom{N-1}{Q-1} F_2(i\omega_n + \Delta_{Q-1,1}, -i\omega_n + \Delta_{Q,-1}) - \binom{N-1}{Q} F_2(-i\omega_n + \Delta_{Q+1,-1}, i\omega_n + \Delta_{Q,1}) \right]$$

$$C_2(Q, P) \equiv \begin{cases} \epsilon(P) \binom{N-2}{Q-2} & \text{if } P^{-1}(1) < P^{-1}(2) \text{ and } P^{-1}(3) < P^{-1}(4) \\ \epsilon(P) \binom{N-2}{Q} & \text{if } P^{-1}(1) > P^{-1}(2) \text{ and } P^{-1}(3) > P^{-1}(4) \\ -\epsilon(P) \binom{N-2}{Q-1} & \text{else} \end{cases}$$

$$C_1(Q, P) \equiv \begin{cases} \binom{N-1}{Q-1} & \text{if } P^{-1}(\{1, 3\}) = \{1, 3\} \\ \binom{N-1}{Q} & \text{if } P^{-1}(\{1, 3\}) = \{2, 4\} \\ 0 & \text{else} \end{cases}$$

$$F_n(\omega_j, j = 1..n) \equiv \int_{\beta > \tau_1 > \dots > \tau_n} \left( \prod_{i=1}^n d\tau_i \right) \exp\left(\sum_{i=1}^n \omega_j \tau_j\right)$$

In these expressions,  $E_Q \equiv U(Q - N/2)^2/2$  are the atomic energy levels,  $\Delta_{Q,a} \equiv E_{Q+a} - E_Q$ ,  $\epsilon$  is the signature of the permutation  $P$ , and we used the notation  $f(x_j, j = 1..4) \equiv f(x_1, x_2, x_3, x_4)$ . We compute  $F_4$  and  $F_2$ , using the relations  $\omega_1 + \omega_2 + \omega_3 + \omega_4 = 0$  and

$\omega_1 + \omega_2 = 0$  respectively. The algorithm can be decomposed into three functions : (i) From  $U$  and  $T$ , compute  $\chi_{nm}$  for  $|n|, |m| < 100$  and then its lowest eigenvalue  $E_0(U, T)$ ; (ii) Find a point  $p_0$  below the instability temperature  $T_i$  and a majoration  $T_M$  of  $\max(T_i)$  and  $U_M$  of  $U_{c1}$ ; define a path in the  $(U, T)$  from  $(0, 0)$  to  $(0, T_M)$  to  $(U_M, T_M)$  to  $(U_M, 0)$ ; (iii) For about 50 points  $p$  on this path, solve for  $E_0(U, T) = 0$  on the line defined by  $p$  and  $p_0$  using a dichotomy. To speed up the computation, the sums over permutations and  $Q$  in  $A$  and  $B$  are expanded automatically into C++ code, which is inlined in the main program. Diagonalisations are performed using

- 
- [1] For a review, see e.g.: M. Imada, A. Fujimori and Y. Tokura, *Rev. Mod. Phys.* **70**, 1039 (1998).
- [2] For a review, see e.g.: O. Gunnarsson, *Rev. Mod. Phys.* **69**, 575 (1996).
- [3] S. Lefebvre, P. Wzietek, S. Brown, C. Bourbonnais, D. Jérôme, C. Mézière, M. Fourmigué, and P. Batail *Phys. Rev. Lett.* **85**, 5420-5423 (2000).
- [4] For a review, see e.g.: Strong Coulomb Correlations in Electronic Structure Calculations, Edited by V. Anisimov. Gordon and Breach (2001)
- [5] W. Metzner and D. Vollhardt, *Phys. Rev. Lett.* **62** 324 (1989).
- [6] A. Georges and Kotliar, *Phys. Rev. B* **45**, 6479 (1992).
- [7] For a review, see: A. Georges, G. Kotliar, W. Krauth and M. Rozenberg, *Rev. Mod. Phys.* **68**, 13 (1996).
- [8] For a review, see: T. Pruschke, M. Jarrell, and J.K. Freericks, *Adv. Phys.* **42**, 187 (1995)
- [9] M. Jarrell, *Phys. Rev. Lett.* **69**, 168 (1992); M. Rozenberg, X. Y. Zhang and G. Kotliar, *Phys. Rev. Lett.* **69**, 1236 (1992); A. Georges and W. Krauth, *Phys. Rev. Lett.* **69**, 1240 (1992).
- [10] X.Y. Zhang, M. J. Rozenberg, and G. Kotliar *Phys. Rev. Lett.* **70**, 1666, (1993); A. Georges and W. Krauth *Phys. Rev. B* **48**, 7167 (1993); M. Rozenberg, G. Kotliar, and X. Y. Zhang *Phys. Rev. B* **49**, 10181 (1994).
- [11] M. Rozenberg G. Kotliar H. Kajueter G. A. Thomas D. H. Rapkine J. M. Honig and P. Metcalf, *Phys. Rev. Lett.* **75**, 105 (1995).
- [12] G. Moeller, Q. Si, G. Kotliar, M. Rozenberg and D.S. Fisher, *Phys. Rev. Lett.* **74**, 2082 (1995).
- [13] G. Moeller, *Ph.D Rutgers*, unpublished.  
<http://www.physics.rutgers.edu/~kotliar/thesis/moeller.ps.gz>.
- [14] G. Kotliar, *Eur. Phys. J. B*, **11**, 27 (1999). G. Kotliar, E. Lange and M.J. Rozenberg, *Phys. Rev. Lett.* **84**, 5180 (2000).
- [15] J. Joo and V. Oudovenko *Phys. Rev. B* **64**, 193102 (2001).
- [16] R. Bulla, *Adv. Solid State Phys.* **40**, 169 (2000); R. Bulla, T. Costi and D. Vollhardt *Phys. Rev. B* **64**, 045103 (2001).
- [17] M. Caffarel and W. Krauth, *Phys. Rev. Lett.* **72**, 1545 (1994); Q. Si, M. Rozenberg, G. Kotliar and A. Ruckenstein, *Phys. Rev. Lett.* **72**, 2761 (1994).
- [18] This applies provided the bare density of states has a sufficiently smooth variation with energy, which is the case of the model d.o.s considered in this paper
- [19] O. Gunnarsson, E. Koch and R. Martin, *Phys. Rev. B* **54**, R11026 (1996).
- [20] J. E. Han, M. Jarrell and D. L. Cox, *Phys. Rev. B* **58**, R4199 (1998).
- [21] M. J. Rozenberg, *Phys. Rev. B* **55**, R4855 (1997).
- [22] B. Amadon and S. Biermann, unpublished.
- [23] G. Kotliar and H. Kajueter, *Phys. Rev. B* **54**, R14221 (1996).  
H. Kajueter and G. Kotliar, *Int. J. Mod. Phys.* **11**, 729 (1997).
- [24] P. Lu, *Phys. Rev. B* **49**, 5687 (1994).
- [25] A. Georges and G. Kotliar, *Phys. Rev. Lett.* **84**, 3500 (2000).
- [26] N. Read and D.M. Newns, *Adv. Phys.* **36** p.799 (1987).
- [27] G. Kotliar and A. Ruckenstein, *Phys. Rev. Lett* **52**, 1362 (1986).
- [28] R. Fresard and G. Kotliar, *Phys. Rev. B* **56**, 12909 (1997).  
H. Hasegawa, *J. Phys. Soc. Jpn.* **66**, 3522 (1997).
- [29] R. Raimondi and C. Castellani, *Phys. Rev. B* **48**, 11453 (1993).
- [30] One should note however that the large- $N$  solution of Sec. III suggests that the temperature above which the metallic solution disappears (spinodal) has a different temperature dependence:  $T \propto (\tilde{U} - \tilde{U}_{c2})^{3/2}$ .